

ABSTRACT OF THE DISCLOSURE

A computational method that predicts chemical and electrostatic properties of residues in proteins and utilizes
5 information contained in those predictions to identify various interaction sites is disclosed. The various interaction sites may include, for example, cofactor binding sites, ligand binding sites, catalytic (active) sites or recognition sites. The method of the invention identifies the ionizable residues in the protein
10 with anomalous predicted titration behavior and searches for the clustering of those residues into putative interaction sites. Practicing the method of the invention requires only the structure of the subject protein (which may be deduced, *a priori*, from the amino acid sequence) and, thus, may be applied to proteins that
15 bear no similarity in structure or sequence to any previously characterized protein.

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